Nanoalloys: From Theory to Applications of Alloy Clusters and Nanoparticles

Riccardo Ferrando, Julius Jellinek, and Roy L. Johnston


Searching for low-energy structures of nanoparticles: a comparison of different methods and algorithms

G Rossi and R Ferrando

Dipartimento di Fisica, Università di Genova and CNR/INFM, Via Dodecaneso, 33, 16146 Genova, Italy

Searching for the optimum structures of alloy nanoclusters†

Riccardo Ferrando,a Alessandro Fortunelli and Roy L. Johnston

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Outline: nanoalloys structure

- Generalities on cluster and nanoalloy structures
- Global optimization problem
- Global optimization strategies
  - Simulated annealing
  - Genetic algorithms
  - Basin hopping
    - Order parameters
    - HISTO algorithm
    - Parallel excitable walkers algorithm
- Examples: AgCu, AgNi, AgPd, PtCo, PtCo/MgO
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**Nanocluster structures**

Crystalline structures: pieces of a bulk crystal (fcc, bcc, hcp....)
For example: take an atom in an fcc crystal together with its 12 neighbours

![Cuboctahedron of 13 atoms](image1)

But there is more
No translational invariance → possibility of **fivefold symmetries**
For example: pack 12 atoms around a central one as tight as possible

![Icosahedron of 13 atoms](image2)

6 fivefold axes, 20 triangular facets
Structural motifs of nanoclusters: guidelines in the search for stable cluster structures

- Crystalline polyhedra
- Non-crystalline polyhedra: Icosahedra and Decahedra
**fcc polyhedra**

**Octahedron:**
two square pyramids with their basis in common

**Truncated octahedron (TO):**
cut the six vertexes of the octahedron to get square and hexagonal facets

**Cuboctahedron:**
a special kind of TO with square and triangular facets
The Mackay icosahedron: predicted theoretically in 1962 by Mackay and observed in the ’70 in argon clusters
Decahedron:
two pentagonal pyramids sharing a common basis

Ino decahedron:
truncate the lateral border to create rectangular facets

Marks decahedron:
truncate the lateral vertexes to create reentrances (Marks, 1985)
Energetics of pure nanoclusters

**Mackay Icosahedra**
- Quasi-spherical shape
- Close-packed surface but strong internal strain:
  - Maximize the number of NN bonds
- Favourable at small sizes

**Marks Decahedra**
- Intermediate case:
  - Favourable at intermediate sizes

**fcc polyhedra**
- Far from spherical shape but no internal strain
- Not many NN bonds but of good quality
- Favourable at large sizes
The sequence of the most favourable structures is:

- icosahedra (Ih),
- decahedra (Dh), and finally
- fcc truncated octahedra.

Crossover sizes depend on the material.

\[ \Delta = \frac{E_{\text{TOT}}(N) - N\varepsilon_c}{N^{2/3}} \]

Alloy nanoclusters (nanoalloys)
Chemical ordering

<table>
<thead>
<tr>
<th>Random solution</th>
<th>Ordered alloy</th>
<th>Core-shell</th>
</tr>
</thead>
<tbody>
<tr>
<td>Three- or multi-shell</td>
<td>Phase separated (Janus particles)</td>
<td></td>
</tr>
</tbody>
</table>
Supported nanoparticles
Wulff-Kaisheew construction

\[
\frac{\Delta h_s}{h_i} = \frac{E_{adh}}{\gamma_i}
\]
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What is the best structure of a nanocluster?

Consider a free nanocluster of given size and composition. What is its minimum-energy structure?

Global optimization of the Potential Energy Landscape

$$U(r_1, \ldots, r_N) \ [= U(x)]$$
Potential Energy Landscapes

funnel 1

funnel 2

funnel 3

funnel 4

Global Minimum (GM) here!

Disconnectivity graphs

Global Minimum (GM) here!

- Single stem representing the funnel of the GM
- 99% of the minima are within two rearrangements of the GM
- The energy needed to reach the GM-linked saddle point is small

[J. P. K. Doye et al., JCP 111 (1999)]
Disconnectivity graphs

- Low energy minima are separated into two main funnels
- The two funnels are separated by a high energy barrier

$\text{LJ}_{38}$

Structure: fcc truncated octahedron (TO)

Global Minimum (GM) here!

[J. P. K. Doye et al., JCP 111 (1999)]
How many local minima on the PES?

The rate of growth of the # of minima vs. size is

- system-dependent
  - different model potentials
  - different parametrizations of the same model

\[ N_{\text{tot min}}(N) = e^{\alpha N} \]

IF subsystems have independent stable configurations, then

\[ N_{\text{tot min}} = N_{\text{min}}(mN) = N_{\text{min}}(N)^m \]

\[ N_{\text{min}}(N) = e^{\alpha N} \]
Local minima on clusters’ PES

Huge number of local minima

Lennard-Jones

\[ N_{\text{min}} \sim e^N \]
NP-hard problems

How hard is locating the global minimum cluster configuration as size increases?

Definitions from computational complexity theory:

- **P problem** - decision problem that can be solved by a computer in an amount of time that is polynomial with respect to the size of the input
- **NP problem** - decision problem whose positive solution can be verified in polynomial time
- **NP-hard problem** – non-decisional versions of the NP-complete problems

The travelling salesman problem is NP-hard

In 1985 Wille and Vennik reduce the two-body PES optimisation to the travelling salesman problem

[Wille and Vennik J Phys A 18 (1985); Greenwood 1999]
Global optimization in nanoalloys

The problem is even worse due to the huge number of homotops.

Homotops are isomers sharing the same geometric structure (neglecting local relaxations) but different chemical ordering.

Neglecting symmetries the number of homotops $n_h$ is

$$n_h = \frac{(N_A + N_B)!}{N_A!N_B!}$$
Hopeless problem????

... finding the optimal solution seems impossible

The main point is to understand what we are interested in

Global optimization is a tool to find

low-energy structural motifs and chemical ordering patterns

As size increases, finding the real global minimum becomes less and less important
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Cluster global optimization strategies

General requirements
• no seeds, no *a priori* information
• being able to identify as many funnels as possible
• being able to locate the lowest minimum within each funnel

Classification
• stochastic or thermodynamic algorithms (simulated annealing, basin hopping)
• purely euristic algorithms (genetic algorithm, taboo search, ant colony...
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Simulated annealing

The system is equilibrated at high temperature, then cooled down.

Drawbacks:

- Very time-consuming
- Depending on the characteristics of the PES, it can easily fail

[Lee et al., PRL 91 (2003); J. Comput. Chem. 18 (1997); PRE (2005)]
Disconnectivity graphs

Structure: fcc truncated octahedron (TO)

- low energy minima are separated into two main funnels
- the two funnels are separated by a high energy barrier

Global Minimum (GM) here!

[J. P. K. Doye et al., JCP 111 (1999)]
Simulated annealing

Lennard-Jones 38

Hard to find by SA; few hours of CPU time...
1 minute by basin hopping
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Genetic algorithms

First proposed in the Seventies, inspired by genetic and evolutionary theories

- each individual cluster is represented by its chromosome:

\[
\{x_1, y_1, z_1, \ldots, x_N, y_N, z_N\} \quad \text{atomic coordinates}
\]

- a \textit{fitness} measures how much an individual matches the final requirements (= having the lowest energy of the PES)
Standard genetic algorithm

Evolution theory

- Population of individuals
- Couple of parents individuals
- Mating: the genetic code of their chromosomes is mixed
- Mutations: light, random perturbation of the genetic codes of the offsprings
- Natural selection: part of the offspring survives, the other individuals die
- A new generation is ready for mating...

Genetic algorithm

- Population of clusters, randomly initialized
- Couples of parents clusters are selected
- Mating operators mix parents’ atomic positions in order to obtain the offspring
- Mutation operators slightly modify atomic positions in the offspring
- Clusters with low energy (= best fitness) are accepted into the new generation. The others are rejected
- A new generation of clusters is ready to be processed by mating
Improvements on standard GA

Jean-Baptiste Lamarck (1744-1829)

*If an organism changes during life in order to adapt to its environment, those changes are passed on to its offspring*

... not right in biology but useful for optimization!

- Offspring cluster, after mutation. Its fitness is not good $\rightarrow$ high probability to be rejected

- Offspring cluster, after mutation and adaptation (= local minimization procedure) $\rightarrow$ better fitness, higher probability to be part of the next generation
n_g = total number of generations
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Basin hopping

*Deformation* methods alter the shape of the PES

- reducing the number of minima
- changing their appearance

Basin hopping: $\tilde{E}(X) = \text{min } [E(X)]$

Moves are accepted/rejected according to a MC-Metropolis rule

Probability to accept $S \rightarrow D$ move:

- $\tilde{E}_D \leq \tilde{E}_S \rightarrow p_{SD} = 1$
- $\tilde{E}_D \geq \tilde{E}_S \rightarrow p_{SD} = \exp\left[-(\tilde{E}_D - \tilde{E}_S)/k_B T\right]$
The Potential Energy Surface and its transformation

\[ p(x) \propto \exp \left[ -\frac{U(x)}{k_B T} \right] \]

Local minimization \[ U'(x) \]

\[ p'(x) \propto \exp \left[ -\frac{U'(x)}{k_B T} \right] \]

Basin hopping is a Metropolis Monte Carlo walk on the transformed PES at constant temperature T
Core algorithm block diagram

\( n_{\text{MC}} = \text{total number of MC steps} \)
Cluster
• N, chemical composition

Potential parametrization
• RGL, 4x3 param; LJ, 2x3 param; metal-oxide, 27x2 param; embedded atom, 3 set of param + spline interpolation

Run configuration
• Seeded/unseeded; move; order parameter yes/no; algorithm (ex: MC-Metropolis)
Core algorithm block diagram

MOVE

Single Shake

Shell Bond

Ball

Exchange

High-temperature Molecular Dynamics
Memory in global optimization

“Memory would seem to be an integral component of any search which deserves to be called intelligent”

Fred Glover

- Energy Landscape Paving [Hansmann PRL 86 (2002)]
- Minima hopping [Goedecker JCP 120 (2004)]

Is it possible to modify the basin hopping approach so as to take into account some memory effect?
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Order parameters

Structural/chemical order parameters (op) are useful to:

• Distinguish among clusters with same energy but different structures/chemical orders

• Monitor what funnels are explored during GO

• Save information about the lowest-energy representatives of different structural families
Order parameters

Structural order parameters (free clusters)

- Common Neighbor Analysis
  Each couple of nearest neighbours (nn) A and B is assigned a triplet \((r,s,t)\), called *signature*

\[ r \text{ is the number of nn common to A and B} \]
\[ s \text{ is the number of nn bonds among the } r \text{ nn} \]
\[ t \text{ is the length of the longest chain one can build with the } s \text{ bonds} \]

On the left: example of \((5,5,5)\) signature
Order parameters

Structural order parameters (free clusters)

- Common Neighbor Analysis

<table>
<thead>
<tr>
<th>N</th>
<th>Structure</th>
<th>(5,5,5) %</th>
<th>(4,2,1) %</th>
<th>(4,2,2) %</th>
</tr>
</thead>
<tbody>
<tr>
<td>13</td>
<td>Ih</td>
<td>28.57</td>
<td>0.00</td>
<td>0.00</td>
</tr>
<tr>
<td>19</td>
<td>double Ih</td>
<td>33.82</td>
<td>0.00</td>
<td>0.00</td>
</tr>
<tr>
<td>38</td>
<td>TO</td>
<td>0.00</td>
<td>41.66</td>
<td>0.00</td>
</tr>
<tr>
<td>55</td>
<td>Ih</td>
<td>10.3</td>
<td>0.00</td>
<td>38.5</td>
</tr>
<tr>
<td>75</td>
<td>Dh</td>
<td>1.25</td>
<td>28.2</td>
<td>20.4</td>
</tr>
<tr>
<td>79</td>
<td>TO</td>
<td>0.00</td>
<td>50.0</td>
<td>0.00</td>
</tr>
<tr>
<td>147</td>
<td>Ih</td>
<td>5.17</td>
<td>17.24</td>
<td>38.79</td>
</tr>
</tbody>
</table>

Table 1. The percentage of (5,5,5), (4,2,1) and (4,2,2) signatures for Ih, Dd and TO magic clusters

Local 5-fold symmetry
Volume fcc symmetry
Stacking faults in fcc lattice
Order parameters

Structural order parameters (supported clusters)
• # of atoms in contact with the surface
• # of nn bonds in the contact layer
Order parameters

Chemical order parameters (binary clusters)
- # of heterogeneous bonds

16  6  22
Block diagram

\( n_{MC} = \text{total number of MC steps} \)

1. **Initialization**
2. **Local Minimization**
3. **Move Selection**
4. **Move**
5. **Local Minimization**
6. **Save**
7. **Recover Old Coordinates**
8. **Stop**
Every time a move is accepted,
• OP value is evaluated
• Minima are classified in the OP space

Block diagram

INITIALIZATION

LOCAL MINIMISATION

MOVE SELECTION

MOVE

LOCAL MINIMISATION

STRUCTURAL ANALYSIS

SAVE

RECOVER OLD COORDINATES

STOP

n=n+1
n=1,…n_{MC}

 accepted

best

not best

n=n_{MC}

not accepted

n=n_{MC}

IF

IF

accepted
Example: $\text{Au}_{90}\text{Cu}_{190}$
Order parameters

Structural/chemical order parameters are useful to:

• Distinguish among clusters with same energy but different structures/chemical orders

• Monitor what funnels are explored during GO

• Save information about the lowest-energy representatives of different structural families

• Help the algorithm to explore as many funnels as possible
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HISTO code

A memory factor within the Basin hopping scheme

- At each step, a histogram in the op space is built to take memory of the explored regions. High histogram bars --> frequently explored regions of the op space.

Initial state $S \rightarrow h_S$
Destination state $D \rightarrow h_D$

Energy is modified:
$\tilde{E} = \min(E) + f(h)$

Acceptance rule becomes:
$p_{SD} = \exp\left[-(\tilde{E}_D - \tilde{E}_S)/k_B T\right]$  

$\rho = $ hetero bonds

HISTO will favor a uniform exploration of the order-parameter space.
3 test clusters
Test

Order parameter: CNA sig(555)
Test

Order parameter: CNA sig(555)

Number of successful opt.

\( \text{LJ}_{75} \)

\( N_s \)

Temperature [K]
Test

Order parameter: hetero nn bonds

Number of successfully opt.

Temperature [K]

$N_s$

$\text{Ag}_{32}\text{Cu}_6$
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Parallel Excitable Walkers code

Parallel search across funnels

Encouraged!  
Discouraged!
Parallel Excitable Walkers code

Order parameter and neighbouring condition

walkers $a$, $b$, $c$
neighbouring condition:
if $|p(b) - p(c)| < \delta \rightarrow E^*_b = E_b + E_{exc}$

Initial state $S \rightarrow h_s$
Destination state $D \rightarrow h_d$

Acceptance rule for $a$ becomes:
$p_{SD} = \exp\left[\frac{-(E_D - E^*_S)}{k_B T}\right]$
Test clusters: $LJ_{38}$ and $Ag_{32}Cu_6-pc_6$
Test

Order parameter: CNA sig(555)
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Alloy nanoclusters (nanoalloys)

Chemical ordering

Random solution
Ag-Pd

Ordered alloy
Pt-Co

Core-shell
Ag-Cu, Ag-Ni

Three- or multi-shell

Phase separated (Janus particles)
Nanoalloys: what is their structure?

Statement of the problem

Given size and composition of the nanoalloy, what is the lowest-energy structure and ordering pattern?
Computational methodology

How to proceed?

Make an “inspired” guess and direct ab-initio relaxation?

... very difficult
too many structures, unexpected geometries

Ab-initio global optimization?

... possible, but limited to small sizes
A possible computational strategy

• Build up an atom-atom interaction potential and define a potential energy surface (PES) $E(\{r\})$

• Search for significant structural families in this PES, and, for each family, build up a database of low-energy structures. Use global optimization and growth simulations.

• Optimize these structures by DFT methods

• .... make “educated” guesses and/or improve the potential and iterate....
Semi-empirical tight-binding approach

\[ E = \sum_j \left( E_j^b + E_j^r \right) \]  \[ \text{[Rosato Phyl. Mag. A 59 (1989)]} \]

\[ E_j^b = -\sqrt{\sum_i \xi_{sw}^2 e^{-2q_{sw} \left( \frac{r_{ji}}{r_{sw}} - 1 \right)}} \]
\[ E_j^r = \sum_i A_{sw} e^{-p_{sw} \left( \frac{r_{ji}}{r_{sw}} - 1 \right)} \]

many-body attractive term \hspace{1cm} \text{two-body repulsive term}

Three sets of four parameters

2 homogeneous, 1 heterogeneous interactions

Parameters fitted to bulk properties

Cohesion energy, lattice parameter, bulk modulus, elastic constants
Ag-Cu and Ag-Ni: non-miscible systems

Ag-Cu bulk phase diagram
wide miscibility gap

Phase Diagram for Copper and Silver at 1 atm
Ag-Cu and Ag-Ni of 38 atoms: composition matters

$\text{Ag}_{38}, \text{Cu}_{38}$ and $\text{Ni}_{38}$ are truncated octahedra

BUT

almost all $\text{Ag}_m\text{Cu}_{38-m}$ and $\text{Ag}_m\text{Ni}_{38-m}$ are not

Ag-Cu and Ag-Ni of size 34 atoms: composition matters again

$\text{Ag}_{27}\text{Cu}_7$, $\text{Ag}_{17}\text{Cu}_{17}$, $\text{Ag}_{12}\text{Cu}_{22}$

Polyicosahedra
built by elementary icosahedra of 13 atoms
Core-shell polyicosahedra

Size 38: the sixfold pancake: $(32,6)\text{plh}^6$

Size 34: the fivefold pancake: $(27,7)\text{plh}^7$
Driving forces for core-shell structures

• Tendency to phase separation in bulk
• Difference in surface energy
• Atomic size mismatch: “big” atoms tend to go outside
• ... but core shell structure are not necessarily with a centered core..
Core-shell polyicosahedra are very stable. Why?

Polyicosahedra maximize the number of bonds at a given size...

.... but bonds are strained in pure polyicosahedra: expanded surface bonds, contracted internal bonds

The bond order – bond length correlation prefers the contrary: contracted surface bonds and longer internal bonds.

Make binary clusters substituting the internal atoms with atoms of smaller size: core shell polyicosahedra

Mismatch: Ag-Cu 12%, Ag-Ni 14%, Ag-Pd 5%
Ag-Cu core-shell chiral icosahedra

Mackay          anti-Mackay          chiral icosahedron

(A)              (B)                (C)

The number of nearest-neighbour bonds increases in the transformation:

A quite general mechanism, valid for AgNi, AgCo, AuNi, AuCo too

Quasi-Janus Ag-Cu nanoparticles

Global optimization:
Cu aggregates in off-center position

Experiment:
off-center Cu aggregate

Ag-Pd phase diagram: miscible system

Ag-Pg bulk phase diagram
solid solutions for all compositions
no long range order
AgPd: Optimization of chemical ordering at fixed geometry

Size 1289 (diameter 3.5 nm) – Ag75%Pd25%

The external shell is 100% Ag !!.

2nd shell enriched in Pd (53%)

Cross section of the cluster: intermixing in the inner part.

R. Novakovic, G. Borzone and R. Ferrando, to be published (2012)
Pt-Co phase diagram: mixing and ordering

Long-range order for several compositions at low temperature

Pt75%-Co25% atomic percentage

Pt50%-Co50% atomic percentage

L$_1$ ordered phase
Pt-Co at 50% - 50% composition

N < 100: polyicosahedra: sixfold pancakes

100 < N < 1000: decahedra

N > 500: fcc (fct indeed) clusters compete with decahedra

Theory: Icosahedra are not dominant even at small size (may be with the exception of few magic numbers)


Experiment:
- Penuelas et al., PRL 100, 115502 (2008): metastable icosahedra transform upon annealing at sizes of 3 nm
Nanoalloys on surfaces
MgO(001) surface

a perfect checkerboard of Mg and O atoms
MgO(001) surface

Metal atoms adsorb on top of oxygen atoms
Exotic Supported CoPt Nanostructures: From Clusters to Wires

Giovanni Barcaro,† Riccardo Ferrando,*,† Alessandro Fortunelli,*,† and Giulia Rossi*

†Molecular Modeling Laboratory, IPCF-CNR, Via Giuseppe Moruzzi 1, Pisa, 56124, Italy and *Dipartimento di Fisica, Università di Genova, Via Dodecaneso 33, Genova, 16146, Italy

Figure 1. Schematic pictures of free polyicosahedral (plh6, top row) and L12 truncated octahedron (TO, bottom row) structures at a composition of Co18Pt20. Top and side views are shown on the left and right side, respectively. The disclination line in the Frank–Kasper plh6 cluster is indicated. Cobalt atoms are displayed in blue, and platinum atoms are in dark gray.
Pt-Co on magnesium oxide (001)

Pt$_{20}$Co$_{20}$ on MgO(001)

The same pancake structure as in free space
Pt-Co on magnesium oxide (001)

Pt$_{26}$Co$_{23}$ on MgO(001)

Tilted pancake with basis
Pt-Co on magnesium oxide (001)

Pt$_{32}$Co$_{32}$ on MgO(001)

Double tilted pancake
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